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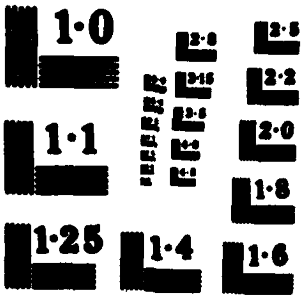
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A RESEARCH PROGRAM FOR THE THEORETICAL STUDY OF THE THERMODYNAMIC AND TRANSPORT PROPERTIES OF DENSE PLASMAS: FINAL REPORT

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A basic theoretical study of the equation of state and transport properties of dense, partially ionized, reacting plasmas has been carried out. This report summarizes the work which is fully described in 14 journal articles, and reports. Topics include

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FINAL REPORT*

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I. INTRODUCTION

Over the past five years, we have pursued a program of theoretical research, partially funded by the Office of Naval Research, on the Equation of State (EOS) and transport properties of dense, partially ionized, reacting plasmas. Although originally motivated by the failure of older, simpler theories[1,2] to describe plasmas produced in new, innovative power sources,[3] this program developed into a far-ranging, multi-faceted study of the basic properties of such complicated systems. Our research efforts, nevertheless, can be divided into three basic categories: 1) Theory of Equation of State and Static Structure; 2) Electrical Conductivity and Dynamic Properties, and 3) Computer Simulation Studies. While these categories are fairly well defined, they are very closely related, and results from each impact on results from the others. Since all of the most significant results have already appeared in published form, the progress made in each of these areas is described only briefly in the following paragraphs. More detailed descriptions can be found in the references listed, by year of publication, in Section III of this report.

*Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48 and supported in part by the Office of Naval Research.

II. MAJOR ACCOMPLISHMENTS

A. Theory of Equation of State and Static Structure

A significant part of our work for ONR involved the development of a fundamental theory of the ionization balance and equation of state of dense, reacting plasmas. Under ONR funding, we were able to extend earlier work on hydrogen and helium to include heavier elements[81a,b]. A detailed tabular EOS (with a polynomial fit provided) was constructed for argon[80a]. Similar, but less detailed, calculations were also carried out for hydrogen, helium, and xenon[83a]. Particular emphasis was placed on the rare gases, because they were anticipated to be the working fluids in the ARTEC MHD power generator.[3]

To facilitate these calculations we had to develop effective potentials to describe the interactions between free electrons and ions with up to fifty-five bound electrons. The model we constructed is mathematically simple, but it still retains the shell structure of the ions[81c].

Another important feature of dense plasmas that we studied was their equilibrium static structure. This is most easily described in terms of the static structure (or form) factors of the plasma. These functions are related to the Fourier transform of the pair distribution function, which gives the probability of finding a pair of plasma particles at a given separation. In weakly coupled plasmas the pair correlations are well described by the Debye-Huckel theory,[4] but for dense plasmas, other methods must be used. Among the most successful of these is an integral equation approximation, known as the Hypernetted Chain(HNC) Equation.[5] This equation has been used to described the classical one-component plasma and molten salts at moderate coupling[80b,c]. For very strong coupling, however, the HNC equation must be improved. We have succeeded in doing this by blending the HNC equation with another integral equation, called the Percus-Yevick equation, in a thermodynamically consistent way. The blended integral equation gives the accuracy of very expensive computer simulations and is no more difficult to solve than the HNC equation[84b,c].

For real plasmas consisting of electrons interacting with ions through an attractive Coulomb potential, direct application of these classical integral equation techniques is impossible, because quantum mechanics is required to prevent the collapse of the system. However, if the density is not too great, the essential quantum mechanics can be incorporated into a pseudopotential which is finite at infinitesimal distances, but behaves like the Coulomb potential at large distances. Using results from our equation of state theory, we have found a suitable method for determining these numerical pseudopotentials from our analytic effective potentials described above. Having accomplished this, we can use the pseudopotentials in the HNC equation to obtain both the static structure and the equation of state properties of real plasmas from the same theory[84a,d].

B. Electrical Conductivity and Dynamic Properties

Our first major success in this area was the calculation of the electrical conductivities of argon and xenon plasmas using a Chapman-Enskog solution[6] to the Gould, Williams, DeWitt(GWD) kinetic equation.[7] These calculations corrected two of the important shortcomings of the usual Spitzer-type theories. First, the relevant statically screened cross sections were calculated from their correct quantum expression. Second, scattering from the electronic shells of the ions and from neutrals was included through the use of analytic effective potentials developed as part of this ONR-sponsored program. These two corrections greatly improved the agreement with Soviet experiments in moderately-coupled, partially ionized plasmas[81d]. Dynamic screening effects were also studied in the context of the GWD kinetic equation[81e], but the results for systems with important short-range contributions to the potential were not as accurate as the Ziman formula[8] or the simple, statically screened results[82a].

We have also studied the relationship between the Ziman[8] and GWD theories of conductivity, and we showed that these apparently different approaches can be obtained from a single, unified approach based on the Green-Kubo theory[9] for the electrical conductivity. The net result of this new approach is a simple expression for the electron-ion collision frequency which depends only on the static structure factors for the plasma[82b]. For modest densities, this theory gives improved agreement over the theory of Spitzer for available experiments on hydrogen plasmas and it also gives good agreement with molecular dynamics simulations of strongly-coupled plasmas[82c].

The new theory described above had the additional advantage that it could be extended to non-zero frequencies to study the conductivity as a function of frequency. Once again, comparison with molecular dynamics results for frequencies below about half the plasma frequency gave excellent agreement. Extending the calculations beyond the plasma frequency, predicted a substantial reduction of the plasma emissivity by short-range correlations[83b].

Our interest in dynamic conductivities required a study of the more general dynamic strucure properties of plasmas. A comparison of several model kinetic equations for the dynamic structure factors has shown that the theory Linnebur and Duderstadt[10] accurately describes the electron peak in the charge-charge structure factor generated in simulation studies[83c]

C. Computer Simulation Studies

We have conducted very detailed and extensive numerical simulation studies of the thermodynamic properties of strongly coupled plasmas. In this work, the Monte Carlo method[11] was used to compute statistical averages over hundreds of thousands of configurations for several hundred ions in thermodynamic equilibrium. The problems we studied included: 1) the classical one component plasma (OCP), consisting of point ions in a uniform background; 2) ionic mixtures; 3) point ions in a polarizable background, and 4) the evaluation of the ion microfield distribution for each of the previous three systems.

For the OCP, we were able to obtain the best estimate, to date, of liquid-solid phase transition[82d], and we obtained very accurate results for the pair distribution function and structure factors. These latter results were very instrumental in our study of the blended integral equation previously described. From our work on ionic mixtures we established a simple and accurate mixing rule for determining the EOS of a mixture from the properties of the indvidual components[84e]. In order to model more realistic systems, we used linear response theory to model the electrons as a polarizable background which screened the ion-ion interactions, and applied this model both to one-component systems and to ionic mixtures[83d].

The observation of spectral lines emitted from plasmas yields important information about the sate of the plasma. As a consequence, we modified our simulation codes to calculate the central ingredient to most theories of plasma line broadening, the distribution of electric microfields around a radiating ion. Our calculations provided the benchmark checks for a new and very efficient theory for the microfield called APEX.[12] This new theory accurately describes the microfield distributions in all three of the plasma models described above[84f].

III. References to ONR Sponsored Research

In this section we list the work we published under ONR sponsorship from 1980 to 1984 by year of publication. These include 14 articles in refereed journals, 4 internal reports, and 2 invited papers.

<u>1980</u>

a. "Equation of State for Self-Excited MHD Generator Studies", F. J. Rogers, M. Ross, G. L. Haggin, and L. K. Wong, LLNL Report, UCID-18557, Feb., 1980.

b. "Improved Equation of State for the Classical One-Component Plasma", W. L. Slattery, G. D. Doolen, and H. E. DeWitt, Phys. Rev. A 21, 2087 (1980).

c. "A HNC Study of Asymmetrically Charged Hard Spheres", F. J. Rogers, J. Chem. Phys. 73, 6272 (1980).

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a. "Equation of State of Dense, Partially Degenerate, Reacting PLasmas", F. J. Rogers, Phys. Rev. A 24, 1531 (1981).

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c. "Analytic Electron-Ion Effective Potentials for $Z \leq 55$", F. J. Rogers, Phys. Rev. A 23, 1008 (1981).

d. "Electrical Conductivity of Dense Plasmas", F. J. Rogers, H. E. DeWitt, and D. B. Boercker, Phys. Lett. 82A, 331 (1981).

e. "Dynamic Screening Effects on Electrical Conductivity in Dense Plasmas", D. B. Boercker, F. J. Rogers, and H. E. DeWitt, LLNL Report, UCID-18574-81-2, Sep., 1981.

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a. "Dynamic Screening of Electron-Ion Collisions", F. J. Rogers and D. B. Boercker, Bull. Amer. Phys. Soc. 27, 1105, (1982).

b. "Electron Collision Frequency in Plasmas", D. B. Boercker, F. J. Rogers, and H. E. DeWitt, Phys. Rev. A 25, 1623 (1982).

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b. "Frequency-Dependent Electrical Conducivity of Strongly-Coupled Plasmas", D. B. Boercker, LLNL Report, UCID-18574-83-2, Dec., 1983.

c. "Dynamic Structure Factors in Two-Component Plasmas", R. Cauble and D. B. Boercker, Phys. Rev. A 28, 944 (1983).

d. "Some Approximate Microfield Distributions for Highly Ionized Plasmas: A Critique", C. A. Iglesias, C. F. Hooper, Jr., and H. E. DeWitt, Phys. Rev. A 28, 361 (1983).

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a. "Integral Equation Method for Partially-Ionized Plasmas", F. J. Rogers, Phys. Rev. A 29, 868 (1984).

b. "New, Thermodynamically Consistent Integral Equation for Simple Fluids", F. J. Rogers and D. A. Young, Phys. Rev. A 30, 999 (1984).

c. "A New, Accurate Statistical Mechanical Theory for Simple Fluids", F. J. Rogers and D. A. Young, Phys. Lett. 102A, 303 (1984).

d. "Statistical Mechanics of Dense Plasmas and Implications for the Plasma Polarization Shift", F. J. Rogers, in Proceedings of the Seventh International Conference on Spectral Line Shapes, Aussois, France, 1984 (in press).

e. "Statistical Mechanics of Light Elements at High Pressure VII: A Perturbative Free Energy for Arbitrary Mixtures of H and He", W. B. Hubbard and H. E. DeWitt (to appear in Ap. J.).

f. "Low-Frequency Electric Microfield Distributions in Plasmas", C. A. Iglesias, H. E. DeWitt, J. L. Lebowitz, and D. MacGowan, (to appear in Phys. Rev. A).

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5. ibid, p. 174.

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